

REPRESENTATION OF MATERIAL ELEMENTS AND GEOMETRY OF SUBSTRUCTURAL INTERACTIONS

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1. INTRODUCTION

This paper collects some characteristic aspects of the general model-building framework of the mechanics of complex bodies, that are bodies in which the material substructure influences prominently the gross behavior through interactions conjugated with substructural changes. Throughout I review critically some results already published in [4], [10], [11] and yet in print [12], [13], and add critical remarks. The emphasis is on issues that are foundational in nature: the geometrical description of the material elements, their energetic characterization, the representation of interactions, conditions for the existence of ground states in conservative setting.

In its primitive meaning, a body can be regarded as an abstract set \mathfrak{B} collecting *material elements*, each one being the smallest piece of matter characterizing the material composing the body. The basic issue is the ‘representation’ of such a set, a representation obtained by mapping \mathfrak{B} in some other set, attributing in this way (geometrical) structure to \mathfrak{B} itself.

In the standard format of continuum mechanics (see the treatises [19], [20]), the geometrical representation adopted is the minimal one: each $\mathfrak{e} \in \mathfrak{B}$ is individuated only by a place x by means of a bijective map k_p from \mathfrak{B} into the three-dimensional space \mathcal{E}^3 (or \mathbb{R}^3 , that is perhaps more convenient for some developments below), with the assumption that the whole \mathfrak{B} is mapped onto a regular region \mathcal{B} which is called *apparent shape* (*place* or *configuration* for short). Regularity is intended here in the sense that \mathcal{B} is assumed to be a bounded domain with boundary $\partial\mathcal{B}$ of finite two-dimensional measure, a boundary where the outward unit normal n is well defined to within a finite number of corners and edges. In this way one considers the generic material element as a windowless box, a *monad* in the words of Leibniz. No information on the shape of the material element, the shape of its internal structure, is accounted for.

However, evidences of condensed matter physics indicate that the material elements are groups of entangled molecules, simple or complex pieces of crystalline structures, stick molecules dispersed in a ground fluid etc., depending on physical circumstances envisaged. In all these cases, when substructural changes determine non-negligible interactions, the standard representation of bodies is too minimalist. The material element is in essence a *system* rather than a windowless box. In representing \mathfrak{B} , then, a map attributing to each material element a *morphological descriptor* of its (inner) substructure has to be defined.

Various choices of the morphological descriptors can be made: Elements of the projective plane may indicate locally the prevailing direction of nematic order in liquid crystals [5]; scalars may be added to account for the degrees of orientation [6], prolation and/or triaxiality [3]. Vectors of the unit sphere S^2 may represent magnetic spins [1]. Second order tensors are measures of independent deformations of macromolecules embedded in a melt [14]. Three-dimensional vectors account for local (random in essence) atomic rearrangements in quasi-periodic alloys [11]. The taxonomy of special models is vast, so is the set of results available in single special cases.

However, in considering such a taxonomy, one becomes aware that to construct the essential structures of these models, at least at the level of first principles such as primitive (weak or strong) balances of actions, it is not necessary to render precise the nature of the morphological descriptor except assuming that it is an element of a finite-dimensional differentiable manifold \mathcal{M} . Consequently, in representing \mathfrak{B} , in addition to the map k_p , another map $k_m : \mathfrak{B} \rightarrow \mathcal{M}$ assigns to each material element the morphological descriptor (often called order parameter) of its substructural shape. Such a point of view has been introduced by G. Capriz in the late 1980's [2].

In general I say that the mechanics associated with maps between manifolds is a unifying setting for existing models of special classes of complex bodies and, above all, a model-building framework for describing the mechanical behavior of exotic material which are sometime the results of new industrial manufactures.

2. TRANSPLACEMENTS AND MORPHOLOGICAL DESCRIPTOR MAPS

Once a reference place $\mathcal{B}_0 := k_{p,0}(\mathfrak{B})$ is selected (for convenience) in \mathbb{R}^3 , any other actual place \mathcal{B} is considered to be achieved in an isomorphic copy $\hat{\mathbb{R}}^3$ of \mathbb{R}^3 itself by means of a *transplacement* map $u := \hat{k}_p \circ k_{p,0}^{-1}$, where $\hat{k}_p := i \circ k_p$, i the isomorphism between \mathbb{R}^3 and $\hat{\mathbb{R}}^3$, so that below $\mathcal{B} := \hat{k}_p(\mathfrak{B})$. The choice of $\hat{\mathbb{R}}^3$ is motivated by the sake of convenience for the developments below. The map $\mathcal{B}_0 \ni x \mapsto u(x) \in \mathcal{B}$ is assumed as usual to be *one-to-one* and *orientation preserving*. Its derivative $Du(x) \in \text{Hom}(T_x \mathcal{B}_0, T_{u(x)} \mathcal{B})$ is commonly indicated by F and is the gradient of deformation.

The inner structure of the material elements is described (at least at a coarse grained level) by a *morphological descriptor map* $\nu = k_m \circ k_{p,0}^{-1}$ with $\mathcal{B}_0 \ni x \mapsto \nu(x) \in \mathcal{M}$ assumed differentiable with spatial derivative indicated by $N := D\nu(x) \in \text{Hom}(T_x \mathcal{B}_0, T_{\nu(x)} \mathcal{M})$.

The map $(u, \nu) : \mathcal{B}_0 \mapsto \hat{\mathbb{R}}^3 \times \mathcal{M}$ then describes the gross deformation and the material substructural morphology. It is convenient to maintain \mathcal{M} as abstract as possible: geometrical structures over it have often a precise physical meaning so that they have to be attributed to \mathcal{M} carefully under the suggestion of specific physical circumstances under scrutiny.

Here I do not consider motions for the sake of brevity, then the natural ambient space for describing the (static) equilibrium behavior of complex bodies is a fiber bundle $(\pi, \mathcal{B}_0, \mathcal{Y})$ with π the canonical projection. I consider maps $\eta : \mathcal{B}_0 \rightarrow \mathcal{Y}$ with $\eta(x) := (x, u(x), \nu(x))$. The first prolongation $j^1(\eta)$ of η is given by

$$(2.1) \quad j^1(\eta)(x) = (x, u(x), F(x), \nu(x), N(x)) = (x, y, F, \nu, N)$$

and is an element of the first jet bundle $J^1 \mathcal{Y}$ over \mathcal{Y} .

The choice of not considering motions leaves out the discussion about the nature of the (independent) kinetic energy that can be attributed (when appropriate) to the material substructures, a discussion in which two aspects play an essential role: (i) the attribution of a metric structure to \mathcal{M} and (ii) the essential *axiom* that the overall kinetic energy admits an additive decomposition into the macroscopic and substructural parts, the latter an axiom used commonly without underlying its essential (foundational) nature.

3. STANDARD AND SUBSTRUCTURAL ACTIONS

Distinct parts of a body interact with each other and with the rest of the environment. Actions are naturally defined as objects power conjugated with the rate of change of places in the case of Cauchy bodies [19], [20]. When material complexity accrues, actions power conjugated with substructural changes have to be accounted for [15].

However, since motions are not considered here, it is necessary to make use of *virtual rates* selected as appropriate vector fields $h \in C(\mathcal{B}_0, \hat{\mathbb{R}}^3)$ and $v \in C(\mathcal{B}_0, T\mathcal{M})$. I consider the pair $\dot{\tau} := (h, v)$ as the rate generated by a semigroup over a space \mathfrak{G} with elements $\tau := (u, \nu)$, a space specified later. Let also \mathfrak{P} be the algebra of *parts* of \mathcal{B}_0 , each representative of it is indicated by \mathfrak{b} .

For any pair $\tau := (u, \nu)$, the generic *power* along (u, ν) is such a map $\mathcal{P} : \mathfrak{P}(\mathcal{B}_0) \times T\mathfrak{G} \rightarrow \mathbb{R}^+$ that $\mathcal{P}(\cdot, \tau, \dot{\tau})$ is additive on disjoint parts and $\mathcal{P}(\mathfrak{b}, \tau, \cdot)$ is linear.

Two key points have to be discussed now: (i) the explicit representation of \mathcal{P} and (ii) its invariance properties with respect to changes in observers. As regards the latter, since any observer is a representation of *all* geometrical environments necessary to describe the morphology of a body and its motion (or ‘sequential’ deformations, when motions are not accounted for), the representation of the manifold of substructural shapes \mathcal{M} must be involved. For *isometric changes in observers* one has to consider the infinitesimal generators of the action of $\hat{\mathbb{R}}^3 \ltimes SO(3)$ over the ambient space $\hat{\mathbb{R}}^3$ and of the same copy of $SO(3)$ over \mathcal{M} , by defining then $h^* := h + c + q \times x$, with $c \in \hat{\mathbb{R}}^3$ and $q \times \in so(3)$, and $v^* := v + \mathcal{A}q$, with $\mathcal{A}(\nu) \in Hom(\hat{\mathbb{R}}^3, T_\nu \mathcal{M})$ so that $\mathcal{A}^*(\nu) \in Hom(T_\nu^* \mathcal{M}, \hat{\mathbb{R}}^3)$. For the sake of brevity I call these changes in observers *semi-classical* and use the word ‘semi’ to remind that the representation of \mathcal{M} is involved.

The explicit representation of the power reflects the way in which one imagines that material elements may interact with each other. If one extends the standard point of view and assumes the existence of bulk and contact actions at macroscopic and substructural levels, a rather natural explicit representation of the *external power* $\mathcal{P}_{\mathfrak{b}}^{ext}(h, v)$ on a generic part \mathfrak{b} , a power measured over (h, v) along (u, ν) , is given by

$$(3.1) \quad \mathcal{P}_{\mathfrak{b}}^{ext}(h, v) := \int_{\mathfrak{b}} (b \cdot h + \beta \cdot v) \, dx + \int_{\partial \mathfrak{b}} (Pn \cdot h + Sn \cdot v) \, d\mathcal{H}^2,$$

with $d\mathcal{H}^2$ the two-dimensional measure, n the normal to $\partial \mathfrak{b}$ in all places in which it is defined. At each x the quantities b and β are elements of $T_{u(x)}^* \mathcal{B} \simeq \hat{\mathbb{R}}^3$ and $T_{\nu(x)}^* \mathcal{M}$ respectively, and represent standard and substructural bulk actions (they

split additively in inertial and non-inertial components when a dynamic setting is accounted for). Standard and substructural contact actions are represented by the first Piola-Kirchhoff stress P and the microstress \mathcal{S} , which are, at each x , elements of $Hom(T_x^* \mathcal{B}_0, T_{u(x)}^* \mathcal{B}) \simeq \mathbb{R}^3 \otimes \hat{\mathbb{R}}^3$ and $Hom(T_x^* \mathcal{B}_0, T_{\nu(x)}^* \mathcal{M}) \simeq \mathbb{R}^3 \otimes T_{\nu(x)}^* \mathcal{M}$, respectively.

Axiom. *At equilibrium the power of external actions is invariant under semi-classical changes in observers, namely*

$$(3.2) \quad \mathcal{P}_{\mathfrak{b}}^{ext}(h, v) = \mathcal{P}_{\mathfrak{b}}^{ext}(h^*, v^*)$$

for any choice of \mathfrak{b} , c and q .

An immediate theorem follows (see also discussions in Section 8 of [11] and in references quoted therein). Below \mathbf{e} indicates Ricci's permutation index.

Theorem 1. (i) *If for any \mathfrak{b} the vector fields $x \mapsto Pn$ and $x \mapsto \mathcal{A}^* \mathcal{S}n$ are defined over $\partial \mathfrak{b}$ and are integrable there, the integral balances of actions on \mathfrak{b} hold:*

$$(3.3) \quad \int_{\mathfrak{b}} b \, dx + \int_{\partial \mathfrak{b}} Pn \, d\mathcal{H}^2 = 0,$$

$$(3.4) \quad \int_{\mathfrak{b}} ((x - x_0) \times b + \mathcal{A}^* \beta) \, dx + \int_{\partial \mathfrak{b}} ((x - x_0) \times Pn + \mathcal{A}^* \mathcal{S}n) \, d\mathcal{H}^2 = 0.$$

(ii) *Moreover, if the tensor fields $x \mapsto P$ and $x \mapsto \mathcal{S}$ are of class $C^1(\mathcal{B}_0) \cap C^0(\bar{\mathcal{B}}_0)$ then*

$$(3.5) \quad Div P + b = 0$$

and there exist a covector field $x \mapsto z \in T_{\nu(x)} \mathcal{M}$ such that

$$(3.6) \quad skw(PF^*) = \mathbf{e}(\mathcal{A}^* z + (D\mathcal{A}^*) \mathcal{S})$$

and

$$(3.7) \quad Div \mathcal{S} - z + \beta = 0,$$

with $z = z_1 + z_2$, $z_2 \in Ker \mathcal{A}^*$.

- The covector z appearing above is a substructural *self-action* within the generic material element. In this sense the field $x \mapsto \nu(x)$ is self-interacting. If one postulates absence of contact interactions of substructural nature, by considering in this way the external power as defined by

$$(3.8) \quad \mathcal{P}_{\mathfrak{b}}^{ext}(h, v) := \int_{\mathfrak{b}} (b \cdot h + \beta \cdot v) \, dx + \int_{\partial \mathfrak{b}} Pn \cdot h \, d\mathcal{H}^2,$$

a theorem analogous to the previous one holds but the last part reads only as follows: There exists a covector field $x \mapsto z \in T_{\nu(x)} \mathcal{M}$ such that $skw(PF^*) = \mathbf{e} \mathcal{A}^* z$ and

$$(3.9) \quad \beta = z,$$

with $z = z_1 + z_2$, $z_2 \in Ker \mathcal{A}^*$. This last equations is less trivial than appearing. In fact, when in non-conservative setting one assumes that z admits an additive decomposition into conservative and dissipative parts (the latter being linear in the rate of the morphological descriptor), then the scheme suggested by (3.9) becomes formally the one of internal variables (see e.g. [18]), differences resting in the circumstance that internal variables are not observable quantities that do not describe internal morphologies

rather the removal from thermodynamical equilibrium. Of course, the two points of view can merge one into the other in appropriate special cases. Take note that, in this case, when $z \in \text{Ker } \mathcal{A}^*$ Cauchy stress $(\det F)^{-1} P F^*$ is symmetric (the condition is sufficient).

- From the theorem above it appears that a crude integral balance of substructural actions, namely the integral version of (3.7), has no geometrical meaning unless \mathcal{M} is embedded in some linear space; contrary, in fact, the integrand would take values in $T^*\mathcal{M}$ which is a non-linear space. Moreover, even when \mathcal{M} is embedded, the integral version of (3.7) does not correspond to any Killing field of the metric in space. Really the significant balance is the *weak balance* of actions

$$(3.10) \quad \mathcal{P}_{\mathfrak{b}}^{ext}(c + q \times x, \mathcal{A}q) = 0, \quad \forall \mathfrak{b} \in \mathfrak{P},$$

a balance accruing directly from the axiom of invariance of the power. The power can be in general written in terms of forms over an appropriate space. A systematic program about the expression of actions in terms of forms has been initiated and developed by R. Segev (see, e.g., [15], [16], [17], and references therein).

4. ENERGY AND THE EXISTENCE OF GROUND STATES

Once the morphology of the generic material element has been represented together with the list of potential interactions it may have with the neighboring fellows and the remaining environment, the local energetic scenario must be specified: it links morphology and representation of interactions. In fact, by the standard use of Clausius-Duhem inequality, one realizes that, at thermodynamical equilibrium, standard and substructural interactions within the body are determined by derivatives of the energy with respect to F , ν , N (see [2]), under the assumption that e be differentiable.

Three cases can be discussed.

- (1) The generic material element \mathfrak{e} is a closed system with respect to its substructure in the sense that (i) there is no migration of substructures leaving \mathfrak{e} , (ii) the material substructure of \mathfrak{e} does not interact energetically with the neighboring fellows.
- (2) The substructure of the generic material element is in energetic contact with the substructures of the neighboring elements. No migration occur.
- (3) The material element is an open system: both energetic contact and migration of substructures are possible.

Of course the classification above is referred to substructural events. At a gross scale, in all cases there are interactions between neighboring material elements considered as a whole, interactions represented by means of standard tensions.

The attention here is primarily focused on item 2 and, in particular, on the case in which only conservative phenomena are involved. They are governed by a 3-form (elastic) energy

$$(4.1) \quad \widehat{\mathfrak{e}} : J^1\mathcal{Y} \rightarrow \wedge^3(\mathcal{B}_0)$$

of the type

$$(4.2) \quad \widehat{\mathfrak{e}} = e \, dx,$$

with e a sufficiently smooth density the dependence of which on state variables is assumed to be given (in isothermal conditions) by

$$(4.3) \quad e := e(x, u, F, \nu, N)$$

so that the global energy $\mathcal{E}(u, \nu)$ of \mathcal{B}_0 is simply

$$(4.4) \quad \begin{aligned} \mathcal{E}(u, \nu) &: = \int_{\mathcal{B}_0} \widehat{\mathbf{e}}(j^1(\eta)(x)) \\ &= \int_{\mathcal{B}_0} e(x, u(x), F(x), \nu(x), N(x)) \, dx. \end{aligned}$$

A pair (u, ν) satisfying the variational principle

$$(4.5) \quad \min_{u, \nu} \mathcal{E}(u, \nu)$$

is called *ground state*. In trying to find minimizers of \mathcal{E} , constitutive assumptions have to be added: (i) the specification of the functional classes in which one places u and ν , (ii) the ‘structural’ properties of e .

- In the case in which the material element is a closed system with respect to its substructure, namely when we are within the setting of item 1 of the list above, e is given by $e := e(x, u, F, \nu)$ so that the energetic contribution of the substructure is purely local. Only the self-action z is present and balances the external bulk action β on the substructure.
- When the generic material element is an open system (item 3 of the list above), one has to consider the substructure as a population of distinct individuals, let say a group of distinct polymeric molecules. Then it is necessary to add another ‘morphological’ information about the world inside the material element, namely the *numerosity* of the substructures, a scalar quantity that satisfies a continuity equation. Moreover, the substructural migration is intrinsically dissipative: it generates a loss of information about the local substructural arrangements, so an increment of configurational entropy and the flux of it is (roughly) proportional by the chemical potential to the flux of the substructures. The chemical potential then increases the list of constitutive entries in (4.3) together with its gradient. The general treatment of this case is presented in [10]: a generalized form of Cahn-Hilliard equation arises and involves a scalar product in the cotangent space of \mathcal{M} .

The energy e admits commonly an additive splitting of the form $e^i(x, F, \nu, N) + e^e(u, \nu)$ where $e^i(x, F, \nu, N)$ is the internal ‘stored’ energy while $e^e(u, \nu)$ is the energy of bulk actions. $e^e(u, \nu)$ splits also in the sum $e_1^e(u) + e_2^e(\nu)$ where $e_1^e(u)$ is the potential of standard bulk (gravitational) forces and $e_2^e(\nu)$ the potential of direct bulk actions over the substructure such as electric fields.

The existence of minimizers for $\mathcal{E}(u, \nu)$ has been discussed by G. Modica and myself in [13]. I review here the essential ingredients of the existence theorem and the theorem itself (or better the main variant of it).

Constitutive assumptions on the functional nature of the fields involved are necessary. Preliminarily, it is helpful to remind that if $u : \mathcal{B}_0 \rightarrow \hat{\mathbb{R}}^3$ is a Sobolev map, that is an element of $W^{1,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$, then $M(Du)$ indicates the 3–vector collecting the minors of Du , i.e. an element of $\Lambda_3(\mathcal{B}_0 \times \hat{\mathbb{R}}^3)$. The n –current integration G_u

over the graph of u is the linear functional on smooth 3-forms ω with compact support in $\mathcal{B}_0 \times \hat{\mathbb{R}}^3$ defined by

$$(4.6) \quad G_u := \int_{\mathcal{B}_0} \langle \omega(x, u(x)), M(Du(x)) \rangle dx,$$

so that $\partial G_u(\omega) := G_u(d\omega)$, $\omega \in \mathcal{D}^2(\mathcal{B}_0 \times \hat{\mathbb{R}}^3)$ (see [8]).

The deformation u is assumed to be a *weak diffeomorphism* (it is written $u \in dif^{1,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$), in the sense that u is considered a $W^{1,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$ map such that (i) $|M(Du)| \in L^1(\mathcal{B}_0)$, (ii) $\partial G_u = 0$ on $\mathcal{D}^2(\mathcal{B}_0 \times \hat{\mathbb{R}}^3)$, (iii) $\det Du(x) > 0$ for almost every $x \in \mathcal{B}_0$, (iv) for any $f \in C_c^\infty(\mathcal{B}_0 \times \hat{\mathbb{R}}^3)$

$$(4.7) \quad \int_{\mathcal{B}_0} f(x, u(x)) \det Du(x) dx \leq \int_{\hat{\mathbb{R}}^3} \sup_{x \in \mathcal{B}_0} f(x, y) dy.$$

In particular, the subspace

$$(4.8) \quad dif^{r,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3) := \left\{ u \in dif^{1,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3) \mid |M(Du)| \in L^r(\mathcal{B}_0) \right\},$$

for some $r > 1$, is of special interest below.

As regards the morphological descriptor maps, constitutive assumptions about the manifold of substructural shapes are first necessary: It is assumed that (a) \mathcal{M} is Riemannian with (at least) C^1 -metric $g_{\mathcal{M}}$, and (b) covariant derivatives are explicitly calculated by making use of the natural Levi-Civita connection. A metric over \mathcal{M} has non-trivial physical meaning with respect to the representation of the (independent) substructural kinetic energy (when it exists) and a consequent influence on the representation of the microstress. Appropriate discussions can be found in [4] and [13]. The connection is crucial in representing the microstress (take note that such a stress is at thermodynamic equilibrium the derivative of the energy with respect to N). If no prevalent role is assigned to the Levi-Civita connection, leaving arbitrary the possibility to select a connection when a specific gauge is not suggested by the underlying physics, even the parallel transport over geodetics over \mathcal{M} would result not only in general non-isometric but even unbounded as a consequence of topological features of \mathcal{M} itself. It is almost trivial to remind that, if a connection would imply an unbounded parallel transport, the representation of the microstress would become meaningless. The C^1 -Riemannian structure (assumption (a) above) implies that \mathcal{M} can be isometrically embedded in \mathbb{R}^N by Nash theorem: it is considered here as a *closed submanifold* in some linear space isomorphic to \mathbb{R}^N for some appropriate N . The use of the Levi-Civita connection implies that the covariant derivative of ν is in agreement with the differential of ν as a map from \mathcal{B}_0 into \mathbb{R}^N . Then the functional assumption about the map ν is that it belongs to the Sobolev space $W^{1,s}(\mathcal{B}_0, \mathcal{M})$, $s > 1$, precisely

$$(4.9) \quad W^{1,s}(\mathcal{B}_0, \mathcal{M}) := \left\{ \nu \in W^{1,s}(\mathcal{B}_0, \mathbb{R}^N) \mid \nu(x) \in \mathcal{M} \text{ for a.e. } x \right\}.$$

In summary, the minimum problem for the energy introduced above is analyzed in the functional class

$$\mathcal{W}_{r,s} := \left\{ (u, \nu) \mid u \in dif^{r,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3), \nu \in W^{1,s}(\mathcal{B}_0, \mathcal{M}) \right\}.$$

Once functional features of the maps u and ν are (constitutively) selected, the energy functional \mathcal{E} is extended to $\mathcal{W}_{r,s}$ by

$$(4.10) \quad \mathcal{E}(u, \nu) = \int_{\mathcal{B}_0} e(x, u(x), Du(x), \nu(x), D\nu(x)) \, dx,$$

where $u(x)$, $Du(x)$, $\nu(x)$ and $D\nu(x)$ are the Lebesgue values of u , ν and their weak derivatives. Assumptions about the structure of the energy e , considered as a map $e : \mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathcal{M} \times M_{3 \times 3}^+ \times M_{N \times 3} \rightarrow \bar{\mathbb{R}}^+$ with values $e(x, u, F, \nu, N)$, are necessary. $M_{3 \times 3}^+$ and $M_{N \times 3}$ represent the space of 3×3 matrices with positive determinant and the one of $N \times 3$ matrices respectively.

- e is assumed to be polyconvex in F and convex in N . More precisely, it is assumed the existence of a Borel function

$$(4.11) \quad Pe : \mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathcal{M} \times \Lambda_3(\mathbb{R}^3 \times \hat{\mathbb{R}}^3) \times M_{N \times 3} \rightarrow \bar{\mathbb{R}}^+,$$

with values $Pe(x, u, \nu, \xi, N)$, which is (i) l. s. c. in (u, ν, ξ, N) for a.e. $x \in \mathcal{B}_0$, (ii) convex in (ξ, N) for any (x, u, ν) , (iii) and also such that

$$(4.12) \quad Pe(x, u, \nu, M(F), N) = e(x, u, \nu, F, N)$$

for any (x, u, ν, F, N) with $\det F > 0$. In this way the energy functional becomes

$$(4.13) \quad \mathcal{E}(u, \nu) = \int_{\mathcal{B}_0} Pe(x, u(x), \nu(x), M(F), N) \, dx.$$

- It is also assumed that e satisfies the growth condition

$$(4.14) \quad e(x, u, \nu, F, N) \geq C_1 (|M(F)|^r + |N|^s) + \vartheta(\det F)$$

for any (x, u, ν, F, N) with $\det F > 0$, $r, s > 1$, $C_1 > 0$ constants and $\vartheta : (0, +\infty) \rightarrow \mathbb{R}^+$ a convex function such that $\vartheta(t) \rightarrow +\infty$ as $t \rightarrow 0^+$.

Rather detailed remarks about the physical nature of the assumptions above, assumptions dealing with the influence of the substructure on the local stability of the material and with the energetic features of the substructural events, can be found in [13]. With the assumptions above, it is now possible to analyze the problem of finding minimizers for \mathcal{E} at least in the case of Dirichlet boundary data. Structure, closure and consequent compactness results in [8] together with the classical Ioffe's semicontinuity result allow one to prove the theorem below.

Theorem 2. [13] *The functional \mathcal{E} achieves the minimum value in the classes*

$$(4.15) \quad \mathcal{W}_{r,s}^d := \{(u, \nu) \in \mathcal{W}_{r,s} \mid u = u_0 \text{ on } \partial\mathcal{B}_{0,u}, \nu = \nu_0 \text{ on } \partial\mathcal{B}_{0,\nu}\}$$

and

$$(4.16) \quad \mathcal{W}_{r,s}^c := \left\{ (u, \nu) \in \mathcal{W}_{r,s} \mid \partial G_u = \partial G_{u_0} \text{ on } \mathcal{D}^2(\mathbb{R}^3 \times \hat{\mathbb{R}}^3), \nu = \nu_0 \text{ on } \partial\mathcal{B}_{0,\nu} \right\}.$$

Above, $\partial\mathcal{B}_{0,u}$ and $\partial\mathcal{B}_{0,\nu}$ are the portions of the boundary where u and ν are prescribed; in particular, the boundary condition $\partial G_u = \partial G_{u_0}$ is a strong anchoring condition (see [8]). On the rest of the boundary, standard and substructural tractions are assumed to vanish. The physical meaning of the boundary conditions for the equilibrium problem of complex bodies has been discussed in detail in [13]. Here I remind only that, although there are shrewdness that allow one to prescribe

in special cases the boundary value of ν , it appears a hard job to imagine some loading device prescribing substructural tractions at the boundary. Consequently, the natural condition could be that the substructural tractions vanish at the boundary.

The existence theorem above is not accompanied by appropriate regularity results. Moreover, a Lavrentiev gap phenomenon is not excluded a priori (see appropriate discussions in [13]; see also [7] and [9]).

Existence results of the type above are also available in terms of varifolds: in this case minimizers may describe fractured states (the relevant work is under completion).

5. FURTHER REMARKS ON STANDARD AND SUBSTRUCTURAL ACTIONS

If the minimizer (u, ν) is of class $C_u^1(\mathcal{B}_0, \mathbb{R}^3) \times C_\nu^1(\mathcal{B}_0, \mathcal{M})$, with \bar{u} and $\bar{\nu}$ the boundary values of the relevant fields along $\partial\mathcal{B}_0$, one may compute the first variation of $\mathcal{E}(u, \nu)$ from the ground state (u, ν) by making use of fields $h \in C_c^1(\mathcal{B}_0, \hat{\mathbb{R}}^3)$ and $v \in C_c^1(\mathcal{B}_0, T\mathcal{M})$. Precisely, if one selects a generic smooth curve $(-1, 1) \ni \varepsilon \mapsto \nu_\varepsilon \in \mathcal{M}$ crossing ν when $\varepsilon = 0$, then v is defined by $v = \frac{d}{d\varepsilon} \nu_\varepsilon|_{\varepsilon=0}$ and $v(x) \in T_{\nu(x)}\mathcal{M}$. By exploiting the first variation $\delta_{h,v}\mathcal{E}$ of \mathcal{E} from the ground state (u, ν) along the direction (h, v) , it is immediate to realize that the map $\varepsilon \mapsto \mathcal{E}(u + \varepsilon h, \nu_\varepsilon)$ is differentiable and the pair (u, ν) satisfies the weak form of Euler-Lagrange equations

$$(5.1) \quad \int_{\mathcal{B}_0} (-b \cdot h + P \cdot Dh + (z - \beta) \cdot v + \mathcal{S} \cdot Dv) \, dx = 0,$$

for any $(h, v) \in C_c^1(\mathcal{B}_0, \hat{\mathbb{R}}^3) \times C_c^1(\mathcal{B}_0, T\mathcal{M})$, with v satisfying the condition $v(x) \in T_{\nu(x)}\mathcal{M}$ above. Moreover, if $(u, \nu) \in C^2(\mathcal{B}_0, \mathbb{R}^3) \times C^2(\mathcal{B}_0, \mathcal{M})$, then (3.5) and

$$(5.2) \quad \text{Div} \mathcal{S} - z + \beta = 0 \quad \text{in } T_\nu^* \mathcal{M}$$

correspond to the Euler-Lagrange equations of $\mathcal{E}(u, \nu)$ with $P := \partial_F e$, $b := -\partial_u e$, $\mathcal{S} := \partial_{D\nu} e$ and $z - \beta := \partial_\nu e$. In particular, by exploiting the additive decomposition of e into internal $e^i(x, Du, \nu, D\nu)$ and external $e^e(u, \nu)$ components, one gets $z := \partial_\nu e^i$ and $\beta := -\partial_\nu e^e$. In this way the specification of the energy eliminates the indetermination in Theorem 1 due to the presence of the term $z_2 \in \text{Ker} \mathcal{A}^*$. Really, such an indetermination can be eliminated (under appropriate smoothness conditions) also by using Noether theorem and requiring covariance, that is invariance of the energy with respect to the action of the group of automorphisms of the ambient space and the action of a Lie group over \mathcal{M} , precisely the group $\text{Aut}(\mathcal{M})$ of automorphisms of \mathcal{M} . This last requirement can be considered as invariance with respect to changes in the ‘representation’ of \mathcal{M} (see [4] in the conservative case and [11] when substructural dissipation occurs only within the generic material element). Special circumstances might require the action over \mathcal{M} of a non-trivial subgroup of $\text{Aut}(\mathcal{M})$.

The issue becomes more complicated when one tries to compute the first variation of \mathcal{E} ‘around’ local minimizers in $\mathcal{W}_{r,s}^d$. In this case, to avoid problems due to the irregularity of minimizers, it is convenient (rather than acting directly on the fields) to make use of horizontal variations induced by maps $\phi \in C_0^1(\mathcal{B}_0, \mathbb{R}^3)$ which determine, for ε sufficiently small, diffeomorphisms $\Phi_\varepsilon(x) := x + \varepsilon \phi(x)$ from \mathcal{B}_0 into itself, diffeomorphisms that leave unchanged $\partial\mathcal{B}_0$. A lower bound

for $Pe(x, u, \nu, M(F), N)$ has to be considered in order to assure coercitivity on $diff^{r, \bar{r}}(\mathcal{B}_0, \hat{\mathbb{R}}^3) \times W^{1, s}(\mathcal{B}_0, \mathcal{M})$, $\frac{1}{r} + \frac{1}{\bar{r}} = 1$, where

$$(5.3) \quad diff^{r, \bar{r}}(\mathcal{B}_0, \hat{\mathbb{R}}^3) := \left\{ u \in diff^{r, 1}(\mathcal{B}_0, \hat{\mathbb{R}}^3) \mid M(D\hat{u}) \in L^{\bar{r}}(\tilde{u}(\mathcal{B}_0)) \right\},$$

and \tilde{u} is the Lusin representative of u . The lower bound is refined with respect to (4.14) in the sense that $\vartheta(\det F)$ is substituted by $|M(F)|^{\bar{r}} \left((\det F)^{\bar{r}-1} \right)^{-1}$, i.e. by an estimate involving the minors of the gradient of the inverse of u , that is the gradient of a L^∞ map \hat{u} defined over $\tilde{u}(\tilde{\mathcal{B}}_0)$, where $\tilde{\mathcal{B}}_0$ is the set of Lebesgue points of both u and Du , and such that both $\hat{u} \circ u = id_{\tilde{\mathcal{B}}_0}$ and $u \circ \hat{u} = id_{\tilde{u}(\tilde{\mathcal{B}}_0)}$, and the right and left multiplication of Du by $D\hat{u}$ gives rise to the identity. The existence of \hat{u} is assured by a structure theorem in [8]. Upper bounds are necessary for Pe and its derivatives to assure that the map $\varepsilon \rightarrow \mathcal{E}_\varepsilon$ be differentiable at zero with derivatives bounded in L^1 . By evaluating the effects of horizontal variations, it follows that (see details in [13]) both $(Du(x))^* \partial_F e$ and $(D\nu(x))^* \partial_N e$ belong to $L^1(\mathcal{B}_0)$, and

$$(5.4) \quad Div \mathbb{P} - \partial_x e = 0$$

in distributional sense, with $\mathbb{P} := eI - F^*P - N^*\mathcal{S} \in Aut(\mathbb{R}^3)$ the extended Hamilton-Eshelby tensor valid for complex bodies (see [4] and references therein).

- Equation (5.4) is the bulk balance of configurational forces in complex bodies in (isothermal) conservative setting. For C^2 fields, (5.4) is not essential for analyzing equilibrium problems; contrary, in presence of evolving bulk defects, a modification of (5.4) including an additional driving force furnishes the evolution equation of the defects themselves. Contrary, the result above (see [8] for a version of it in the standard non-linear elasticity of simple bodies) points out that (5.4) is in a sense more essential than expected because, for irregular minimizers, it furnishes information about the balance of actions in absence of the Lagrangian representation of the balance of the standard forces, namely (3.5).
- Notice that the self force z does not appear in (5.4) explicitly. When dissipative substructural effects accrue within the generic material element, z admits additive decomposition in conservative and dissipative components. In this case only the dissipative part of z , namely z^d , appears in the relevant version of (5.4) as an additive term of the type N^*z^d (see [11], [12]).
- In the case of irregular minimizers, information on substructural interactions and their balance can be obtained by maintaining \mathcal{B}_0 and $\hat{\mathbb{R}}^3$ fixed and altering the manifold of substructural shapes by means of the action of its group of automorphisms $Aut(\mathcal{M})$. Precisely, one selects smooth curves $\varepsilon \rightarrow \bar{\phi}_\varepsilon \in Aut(\mathcal{M})$, with $\bar{\phi} \in C^1(\mathcal{M})$, and defines $\nu_\varepsilon := \varphi_\varepsilon(\nu)$, by indicating by ξ the derivative $\frac{d}{d\varepsilon} \nu_\varepsilon|_{\varepsilon=0}$. Upper and lower bounds mentioned above assure that [13] (i) the map $\varepsilon \rightarrow \mathcal{E}(u, \nu_\varepsilon)$ is differentiable at $\varepsilon = 0$, (ii) \mathcal{S} belongs to $L^1(\mathcal{B}_0, \mathbb{R}^{3*} \otimes T^*\mathcal{M})$ and (iii) the weak balance

$$(5.5) \quad \int_{\mathcal{B}_0} \mathcal{S}(x) \cdot D\xi(x) \, dx + \int_{\mathcal{B}_0} (z - \beta)(x) \cdot \xi(x) \, dx = 0,$$

holds for every $\xi \in C^0(\mathcal{B}_0, T\mathcal{M})$.

- In summary, for irregular minimizers the distributional balance of configurational forces and the weak balance of substructural interactions are the

balances that can be computed in Lagrangian (referential) representation. The Eulerian (actual) version of the weak balance of standard forces can be also computed (see [8], [13]).

The list of interactions and their possible balances does not end here. When discontinuity surfaces and line defects occur within a body and are structured in the sense that they carry own surface and line energy, respectively, surface and line interactions accrue. Their link with surface and line energies is discussed in [4], [11], [12] together with their balances and the invariance properties they satisfy. I remind briefly here the sole case of a smooth coherent structured discontinuity surface Σ which crosses the body and is oriented by a normal vector field $x \mapsto m := m(x)$, $x \in \Sigma$. In referential representation, along a pair (u, ν) , a surface standard stress $\mathbb{T} \in \text{Hom}\left(T_x^*\Sigma, T_{u(x)}^*\mathcal{B}\right)$, a surface microstress $\mathbb{S} \in \text{Hom}\left(T_x^*\Sigma, T_{\nu(x)}^*\mathcal{M}\right)$ and a surface self force $\mathfrak{z} \in T_{\nu(x)}^*\mathcal{M}$ occur along Σ , the first two stresses are presumed a priori, the existence of \mathfrak{z} can be proven by means of $SO(3)$ invariance arguments. Under appropriate smoothness assumptions they satisfy the surface balances

$$(5.6) \quad [P]m + \text{Div}_\Sigma \mathbb{T} = 0,$$

$$(5.7) \quad [\mathcal{S}]m + \text{Div}_\Sigma \mathbb{S} - \mathfrak{z} = 0,$$

where $[\cdot]$ denotes the jump of the relevant quantity across Σ and Div_Σ denotes the surface divergence. Invariance properties of them have been discussed in [4]. The surface standard and substructural actions listed above concur in the surface counterpart of (5.4) together with the surface energy which is commonly assumed to be a function of m , the surface derivative of u , the surface derivative of ν and ν itself, when ν is continuous across Σ . In this equation (which I do not report here) only the dissipative part of \mathfrak{z} appears, when it exists. The conservative part of \mathfrak{z} is absent. Relevant proofs can be found in [4] and [11].

Acknowledgements. This paper is an extended version of a talk I delivered in August 2006 at Madrid, during the ICM 2006. I wish to thank Gianfranco Capriz, Giuseppe Modica and Lev Truskinovsky for deep discussions on the matter we had at Pisa, Firenze and Palaiseau, respectively. My gratitude goes also (last but not least) to Mirek Šilhavý not only for discussions we had but also for inviting me to contribute this paper. The support of GNFM-INDAM and MIUR (the latter through the grant 2005085973—“*Resistenza e degrado di interfacce in materiali e strutture*”—COFIN 2005) is acknowledged. I thank also the “Centro di Ricerca Matematica Ennio De Giorgi” of the “Scuola Normale Superiore di Pisa” for providing an adequate environment for scientific interactions.

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